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1 Abstract

This reports a program of basic research concerned with theoretical studies of combustion and related flow problems that are relevant to the Air Force mission. Of particular focus is work on combustion problems relevant to solid-propellant rockets, of interest to the Propulsion Directorate.

Topics that have been examined include heterogeneous propellant flame modeling, the construction of 1-dimensional flame models from subgrid 3-dimensional descriptions, aluminum agglomeration, the combustion of heterogeneous propellants containing aluminum, the use of a genetic algorithm to optimally define false-kinetics parameters in propellant combustion modeling, the calculation of fluctuations above a burning propellant and the effect of these fluctuations on the turbulent chamber flow, the 1-dimensional combustion of fine aluminum and ammonium perchlorate in fuel binder, the combustion of model propellant packs of ellipses and ellipsoids, and the packing of pellets relevant to igniter modeling.

Other topics are the instabilities of smolder waves, premixed flame instabilities in narrow tubes, and flames supported by a spinning porous plug burner.

Much of this work has been reported in the high-quality archival literature such as the Journal of Fluid Mechanics, the Proceedings of the Combustion Institute, and Combustion Theory and Modelling.

2 Personnel

John Buckmaster, PI
T.L.Jackson, consultant

3 Summary of completed research

Much of our effort was concerned with the modeling of flames supported by heterogeneous rocket propellants and the modeling of the propellants themselves. We have reported in previous grant periods on a number of ground-breaking contributions that we have made to this subject, and significant new progress has been achieved during the grant period reported here.

Our first work on heterogeneous propellant combustion used a 2-step kinetics model, but this was replaced with a 3-step kinetics model which gives improved agreement with experiental data for burning rates of a variety of heterogeneous propellants. This work is publshed:

'New kinetics for a model of heterogeneous propellant combustion', L.Massa, T.L.Jackson, J.Buckmaster *Journal of Propulsion and Power* 21(5), 914-924, 2005. Its abstract is:

In earlier work we describe an unsteady, three-dimensional, phase-coupled combustion code which, with the use of a random packing algorithm to construct model propellants, and the use of a homogenization strategy to account for unresolvably small propellant particles, can be used for the simulation of heterogeneous propellant combustion. This work uses a simple two-step kinetic model for ammonium perchlorate (AP) - hydroxyl terminated polybutadiene (HTPB) combustion which fails to accurately predict variations in the burning rate with AP concentration for a homogenized AP/HTPB blend supporting a one-dimensional flame. Here we describe a three-step model, one which captures the three flames of the Beckstead-Derr-Price (BDP) combustion model, and show that kinetic parameters can be adopted so that one-dimensional AP burning rates and one-dimensional AP/HTBP blend burning rates can be correctly predicted. We discuss *the stability of the underlying flame structures, and highlight a difficulty that arises in these instability-prone systems when simple kinetic models are used to describe them. The combustion model, with the new kinetics, is used to reexamine the burning of random packs, and improved agreement with the experimental burning rates of Miller packs is demonstrated. We also reexamine the problem of sandwich-propellant combustion, and investigate the trend in surface shape and burning-rate variations with pressure and binder width. These trends are compared with experimental results of Price. The sandwich configuration is used to measure the importance of the primary diffusion flame of the BDP model.*

We doubt that better agreement with Miller's results could be achieved, and in that sense this paper is a capstone achievement.

Aluminum is often used as an additive in heterogeneous propellants, and one of the most vexing issues for rocket builders is aluminum agglomeration. This refers to the clustering of aluminum particles at the propellant surface prior to detachment. Substantial nozzle scouring and the generation of an identifiable wake are unwanted consequences. We have been able to use the tools that we have developed to examine this problem in a much more sophisticated fashion than hitherto, and the following paper has been published:

T.L.Jackson, F.Najjar, J.Buckmaster. 'New aluminum agglomeration models and their use in solid-propellant-rocket simulations'. *Journal of Propulsion and Power* 21(5) 925-936, 2005. Its abstract is:

Random packs of ammonium perchlorate and aluminum particles in fuel binder, of the kind used to mimic the morphology of heterogeneous propellants, define distributions of aluminum particles which can be used as the starting point of agglomeration studies. The goal is to predict the fraction of aluminum that agglomerates, and the size distribution of the agglomerates. Three phenomenological models are described, each with one or two parameters that can be adjusted to fit experimental data, and a number of such fits are attempted. It is shown that the agglomeration models can be calibrated to match a wide variety of propellant outputs, as needed for the numerical simulation of rocket chamber flows with aluminum injection. Results for such flows are presented and provide information about the distribution of the aluminum droplets and of the alumina smoke particles that arises from its presence.

In addition to the agglomeration study of aluminum, we have developed a 3-dimensional combustion code to model propellant combustion in the presence of aluminum particles. A key advance over the non-aluminized work is the necessary use of a sophisticated level-set strategy. The following paper has been published:

X.Wang, T.L.Jackson, J.Buckmaster. 'Numerical simulation of the three-dimensional combustion of aluminized heterogenous propellants'. Proceedings of the Combustion Institute, 31, 2006, 2055-2062. Its abstract is:

We report the first 3-dimensional simulations of aluminized propellant combustion, accounting for heat conduction in the solid, combustion in the gas-phase, and coupling of these via the irregularly moving propellant surface, one that can not be defined by a single-valued height function. The simulations are used to examine the dynamics of aluminum particles in the near-neighborhood of the surface after detachment, and to provide an estimate of the time to ignition of the particles, and their speed and height above the surface at ignition. In addition we examine the temperature history of the particles during their rise to the surface, determine whether they melt or not, and in this way test Cohen's well-known melting criterion. And we discuss a simple model which provides insights into how aluminum particles floating on a binder melt layer would migrate because of surface tension effects, and calculate an average migration distance that is consistent with previous agglomeration studies.

All of our propellant work to date has been concerned with AP/HTPB propellants, with or without aluminum. We are interested in examining other ingredients, including, most importantly, HMX. A major difficulty in the modeling is the specification of the parameters in the global kinetics models that are necessarily used. We have developed an optimization strategy that makes use of a genetic algorithm to deal with this difficulty. The following paper has been published:

L.Massa, T.L.Jackson, J.Buckmaster. 'Optimization of global kinetics parameters for heterogeneous propellant combustion using a genetic algorithm'. Combustion Theory and Modelling, 11(4), 2007, 553-534. Its abstract is:

We examine the combustion of heterogeneous propellants for which, necessarily, the chemical kinetics is modeled using simple global schemes. Choosing the parameters for such schemes is a significant challenge, one that, in the past, has usually been met using hand-fitting of experimental data (target data) for global burning properties such as steady burning rates, burn-rate temperature sensitivity, and the like. This is an unsatisfactory strategy in many ways. It is not optimal; and if the target set is large and includes such things as stability criteria, or bounds, difficult to implement. Here we discuss the use of a general optimization strategy which can handle large data sets of a general nature. The key numerical tool is a genetic algorithm that uses MPI on a parallel platform. We use this strategy to determine parameters for AP/HTPB propellants and HMX/HTPB propellants. Only 1-dimensional target data is used, corresponding to the burning of pure AP (HMX) or a homogenized blend of fine AP (HMX) and HTPB. The goal is to generate kinetics models that can be used in the numerical simulation of 3-dimensional heterogeneous propellant combustion. The *results of such simulations will be reported in a sequel.*

Our (small) interest in smolder combustion survives. In work reported in the previous funding cycle on "edge-flames" in smolder we observed instabilities, and so have examined the stability question. The following paper has been published:

Z.Lu, J.Buckmaster, M.Chen, L.Massa. 'Instabilities of reverse smolder waves', Combustion Theory and Modelling, 10(3), 2006, 515-534. Its abstract is:

We use numerical strategies to examine the stability of reverse smolder waves in the context of a model that can permit both fuel-rich and fuel-lean waves. The steady-state response for such waves, maximum temperature versus blowing rate, is characterized, for increasing blowing rate, by a fuel-rich branch of rising temperature followed by a fuel-lean branch of falling temperature, followed by quenching. The propagation speed at the quenching point is nonzero. For the parameters that we consider, the entire fuel-rich branch is unstable to 2-dimensional disturbances, but the dynamic consequences are modest. An interval of the fuel-lean branch whose left boundary is at the point of stoichiometry is stable, but the remainder of the branch, all the way to the quenching point, is unstable. These instabilities are destructive, and the contiguous smolder wave becomes fragmented. Tribrachial fragments can emerge, analagous to the tribrachial or triple flames familiar from gaseous edge-flame studies. Their emergence is characterized by a sharp rise in the maximum temperature, a rise that could lead to a transition to flaming (gas-phase) combustion.

When a heterogeneous propellant is burnt, significant fluctuations in velocity and temperature occur above its surface. These are carried into the chamber and provide boundary conditions for the turbulent chamber flow. The nature of these fluctuations, including the statistics, have not been examined before, but we have done so in the following paper, published in the Journal of Fluid Mechanics.

L.Massa, T.L.Jackson, J.Buckmaster, F.Najjar. 'Flluctuations above a burning heterogeneous propellant'. Journal of Fluid Mechanics, 2007, Vol.581, 1-32. Its abstract is:

A numerical description of heterogeneous propellant combustion enables us to examine the spatial and temporal fluctuations in the flow field arising from the heterogeneity. Particular focus is placed on the fluctuations in a zone intermediate between the combustion field (where reaction is important) and the chamber flow domain, for these define boundary conditions for simulations of the turbulent chamber flow. The statistics of the temperature field and the normal velocity field are described, and characteristic length scales and time scales are identified. The length scales are small compared to any relevant length scale of the chamber *flow, and so the boundary conditions for this flow at any mesh point are statistically independent of those at any other mesh point. But the temporal correlations at a fixed point are significant, and affect the nature of the chamber flow in a variety of ways. We describe the fluctuations in the head-end pressure that arise because of them, and contrast these results with those calculated using a white-noise assumption.*

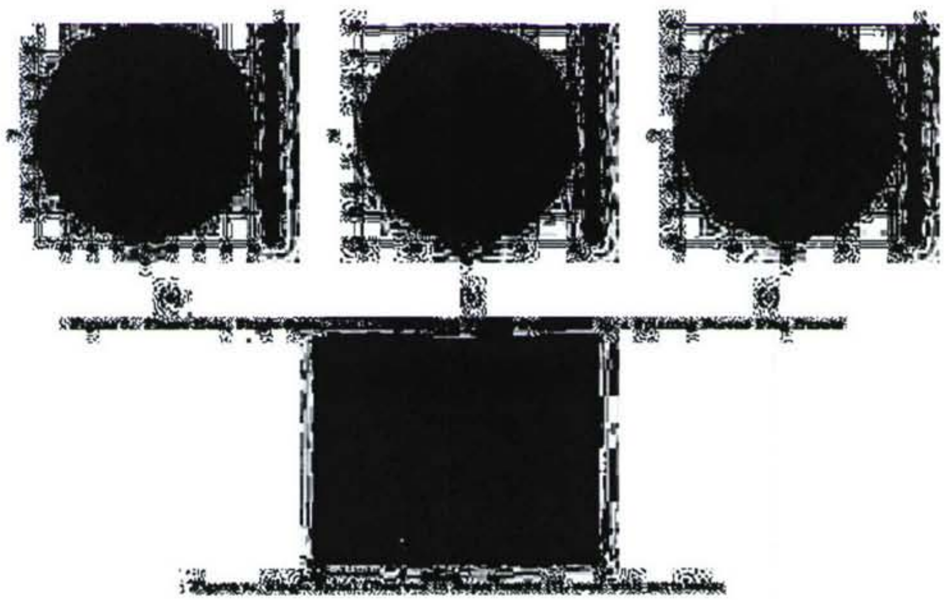

Figure 1: Flames on a spinning burner. The upper row shows simulations, revealing a hole, a single spiral, and a double spiral; the lower figure is a single spiral seen in experiments.

Kishwar Hossain, a privately supported PhD student has been advised by Buckmaster and Jackson, and has been working on a project entitled:

Three-dimensional numerical simulation of flames supported by a spinning porous plug burner'. An abstract for this work is:

A three-dimensional numerical study is undertaken to analyze the characteristics of flames supported by a spinning porous plug methane burner. These flames are characterized by multi-dimensional instabilities at near extinction conditions. The instabilities appear in the form of holes and spirals as observed in experimental studies. The non-uniform flames are simulated numerically (a three-dimensional problem) for Damköhler numbers on the upper branch of the S-response curve close to the extinction point. The flames are analyzed to determine the mechanism of pattern onset, and to gain an understanding of the dynamics of the system.

We believe that this study is relevant to the issue of how diffusion flames behave in turbulent flows. Hossain expects to get a January 2008 degree, and at some time before then a paper will be prepared for publication. A sample figure is shown on the previous page.

A project that was initiated this past year is concerned with the modeling of igniters. We are particularly concerned with igniters in which the energetic material is in the form of short cylindrical rods, and for modeling purposes it is necessary to construct packs of such objects. This has led us also to examine the possibility of packing arbitrarily shaped bodies, rather than the spheres and spheroids that we have previously examined. This is a difficult problem, incomplete at the present time. Shown here is a figure of a pack of cylinders. The maximum packing fraction achieved so far is approximately 50% (beyond that, the code stops). This is a substantial advance over our first efforts which could only generate a 30% packing fraction. We believe that the difficulties are surmountable, and should resources become available at some future date, it will be possible to create suitably dense packs.

We were attracted to some experimental work presented at the 30th Symposium on Combustion (August 2004, Chicago) which reported some interesting flame instabilities in narrow tubes. There is a great deal of interest on flames in narrow tubes these days because of their relevance to micro-combustors, possible replacements for conventional batteries. The following paper was accepted for presentation at the 31st Symposium, and for publication in the Proceedings:

T.L.Jackson, J.Buckmaster, Z.Lu, D.C.Kyritsis, L.Massa. 'Flames in narrow circular tubes'. Proceedings of the Combustion Institute, vol. 31, 2006, 955-962.

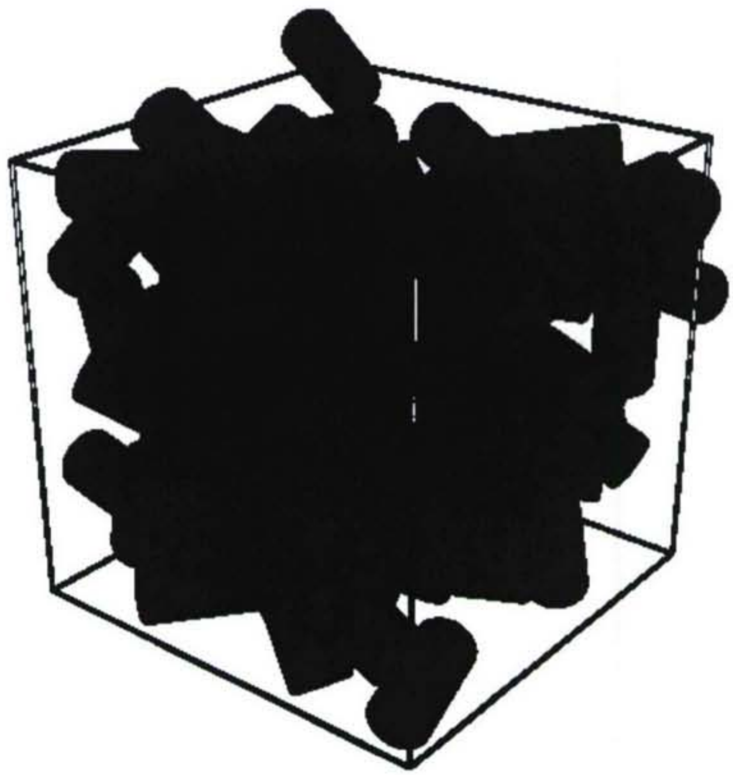

Figure 2: A pack of perforated pellets

We examine an axi-symmetric deflagration located in a tube with thermally active walls. It is noted that the flame-in-tube configuration defines a classical edge-flame, a flame in a shear flow for which there is a water-shed solution for a critical value of the Damköhler number (D)*, ignition front solutions for larger values of* D*, and failure wave solutions for smaller values. We examine semi-infinite tubes with a heat flux imposed at the tube wall ends, to simulate experiments reported in the 30th Symposium. We identify parameters for which stable solutions are obtained at certain flow rates, but unstable solutions are generated at higher flow rates, followed by stable solutions at still higher flow rates. These solutions are consistent with the experimental record. Instability leads either to regular oscillations or to a violent process characterized by quenching and re-ignition.*

Our propellant work has exclusively used model propellant packs in which the oxidizer particles (such as ammonium perchlorate) are represented by spheres of various diameters. Since real particles are not spherical we have long been concerned that this could introduce errors. For this reason we examined the combustion of packs for which the particles are either ellipses (2-dimensional) or spheroids (3-dimensional). The following paper has been published:

X.Wang, J.Buckmaster, T.L.Jackson. 'The burning of ammonium-perchlorate ellipses and spheroids in fuel binder'. Journal of Propulsion and Power, vol.22(4), July-August 2006, 764-768.

Our simulations of heterogeneous propellant combustion have always assumed that the oxidizer particles (ammonium perchlorate) are disks (2-D) or spheres (3-D). Here the effects on the burning rate are examined when the disks/spheres are replaced by ellipses/ellipsoids. In two dimensions, it is shown that an area-preserving deformation of a pack of disks, generating a pack of ellipses, can lead to significant variations in the burning rate. But if the ellipses are randomly packed, so that the alignment of their axes is random, the shape effect is small. In three dimensions, volume preserving deformation which generates ellipsoids leads to burning rate changes no greater than those in two dimensions. Absent a random packing algorithm for ellipsoids, we speculate that here also a random alignment of the axes would eliminate the effect.

There is a great deal of interest in using very fine aluminum in aluminized propellants, particles whose diameters are on the scale of microns. Such small particles, present in large numbers, can not be resolved numerically since the perchlorate particles, as well as larger aluminum particles have diameters that are at least in the tens of microns range. For this reason a homogenized treatment of fine aluminum particles is needed, and we have written a paper which examines the 1-dimensional combustion of binder, fine perchlorate and fine aluminum. This has been published.

T.L.Jackson, J.Buckmaster, X.Wang. 'The modeling of propellants containing ultrafine aluminum'. Journal of Propulsion and Power, 23(1), 2007, 158-165.

In the study of heterogeneous propellants that contain large amounts of fine aluminum and ammonium perchlorate, it is appropriate to distinguish between the matrix - a homogenized blend of fine particles and binder - and larger particles which are embedded in this matrix. Then the burning properties of a pure matrix are required. We construct a 1-dimensional model for this purpose. Key ingredients include the determination of the thermal conductivity and pyrolyis law of the matrix, and an accounting of the radiation field generated by the fine aluminum in the gas phase. Experimental results of Dokhan, Price, Seitzman, and Sigman are used for calibration, and in comparisons.

4 Public Service

The PI is on the editorial board of the journal *Combustion Theory and Modelling*. T.L.Jackson is on the editorial board of the *AIAA Journal.*

5 Honors of T.L. Jackson

Associate Fellow, AIAA, 2006

6 Honors of J.Buckmaster

- Senior U.S. Scientist Award (Humboldt Prize), 1985, 1986
  Alexander von Humboldt Foundation, Germany
- JSPS Fellow, 1986
  Japan Society for the Promotion of Science, Japan
- Fellow, American Physical Society, 1986
  American Physical Society, USA
- Guggenheim Fellowship, 1990
  Guggenheim Foundation, USA
- Fellow of the Institute of Physics (UK), and Chartered Physicist, 1999
- AIAA Propellants and Combustion Award for 2002, "for outstanding theoretical contributions to the physical understanding of fluid mechanics in combustion processes ranging from detonation physics to propellants", 2002
  American Institute of Aeronautics and Astronautics, USA
- Zeldovich Gold Medal of the Combustion Institute for 2004, "for outstanding contribution to the theory of combustion".

7 Other activity

The PI is a participant in a DOE ASCI center, concerned with solid propellant rocket motors, centered in the Computer Science and Engineering program of the University of Illinois. He provides guidance in the context of propellant flame physics and chemistry. His collaborative work with T.L.Jackson, a senior research scientist in the center, comes about because of this.